Influence of Reactor Configuration/Type on the Composition of Mild Gasification Liquids*

M. Rashid Khan
Texaco Research Center, Texaco Inc.
P.O. Box 509, Beacon, NY 12508

Kalkunte S. Seshadri
EG&G Washington, Morgantown, WV 26505

INTRODUCTION

Yield, quality, and the composition of coal liquids produced by devolatilization depend on the reactor configuration, pyrolysis temperature, and on the coal type used. In this investigation a fixed-bed, a fluidized-bed, and an entrained-flow reactor were used in which Pittsburgh No. 8, Illinois No. 6, and Montana Rosebud coals were pyrolyzed. In addition to the above-mentioned reactor configurations, the liquid produced in the fixed-bed reactor was passed through a reactor tube maintained at 500°C and then the sample was collected to investigate the effects of heat treatment on liquid composition/quality. Vapor phase reactions occurring in the pyrolysis liquids are an important consideration keeping in mind that in a mild gasification process, liquid may experience some hot or high-temperature surfaces.

The goals of this study were (a) to understand the chemical reactions induced in the thermal (tube) reactor and (b) to compare compositional differences of coal liquids produced in a fixed-, fluidized-, and entrained-flow reactors. To this end, devolatilization products were separated using gravity-flow liquid chromatography according to chemical functionality. Subsequently, the first fraction which contained mainly neutral aromatic compounds and the third fraction which was composed of phenolic compounds were analyzed using FIMS.

EXPERIMENTAL

The experimental procedure for coal pyrolysis liquid in a fixed-bed reactor is described by Khan (1). In this configuration liquids were generated at 500°C from the Pittsburgh No. 8 and Montana Rosebud coals. In a separate experiment, coal liquids thus generated were passed through a reactor tube (modified configuration) maintained at 500°C before the final collection. In addition, coal liquids from the pyrolysis of Illinois No. 6 coal in a fixed- and a fluidized-bed reactor at 500°C, of Pittsburgh No. 8 coal in a fixed-bed and an entrained-flow reactor at 650°C, and finally, of Pittsburgh No. 8 coal in an entrained-flow reactor at a reactor temperature of 850°C are included in this study. All experiments were performed in an inert atmosphere.

Open column liquid chromatographic (LC) separation was carried out on silica column with sequential elution of the sample with solvents of different polarity (2,3). Field ionization mass spectral data were obtained at SRI International (Menlo Park, California). Data in the tabular form spread over 14 columns contained relative intensity for each mass number. For each spectrum the relative intensities were normalized to 10,000. Details of instrumentation and data acquisition procedure are described by St. John, et al. (4). Data were reduced to identify homologous

*Work reported here was performed at Morgantown Energy Technology Center series in each column and their relative concentration was expressed in mole percent of given fraction or of the total sample. Proton NMR spectra of the Pittsburgh No. 8 coal liquid from the fixed-bed and entrained-flow reactor (reactor temperature 850°C) were obtained at The Energy and Mineral Research Center in Grand Forks, North Dakota, from which average molecular parameters were derived (5). Elemental analysis for these samples were obtained in our laboratory.

RESULTS AND DISCUSSION

Comparison of Coal Liquids Produced in the Fixed-Bed and the Modified Fixed-Bed Reactors

The relative quantities of chromatographic fractions in Pittsburgh No. 8 and Montana Rosebud coal liquids produced in the fixed-bed reactor and in the modified configuration are given in Table 1. The separation results suggest certain gross compositional changes in liquids produced in the modified configuration relative to the raw liquids. The relative weight percent of the residue, which is mainly asphaltenes like materials are less abundant in the liquids produced in the modified reactor, whereas that of fraction 3 is higher than in the raw liquid. These two observations suggest that heavier polar compounds with multifunctional groups are cracked producing simple phenols. On the other hand, FIMS data for the first and the third fractions give details of certain chemical reactions induced in the tube reactor.

In our LC separation the first fraction is composed of alkanes, cycloalkanes, olefins, and neutral aromatic compounds whereas, the third fraction is made up of simple phenolic compounds. FIMS data for these two fractions were reduced to identify homologous series in compound class types mentioned above, using the procedure described by Whitehurst, et al. (6). Results are given in Tables 2 and 3.

According to the separation results one of the reactions in the modified fixed-bed reactor is the formation of simple phenols from heavier polar compounds. FIMS results agree with this conclusion; more importantly, they suggest that two parallel reactions are taking place involving phenols. One is the deoxygenation of simple phenolic compounds such as phenols, naphthols, and others; the other is the formation of hydroxy hydroaromatic and aromatic compounds with three or more condensed rings and hydroxy indenes and benzofurans. Results of elemental analysis (Table 4), however, indicate that there is a decrease in elemental oxygen upon thermal treatment. The decrease in elemental oxygen is consistent with the separation as well as FIMS results. When simple phenols are deoxygenated, the decrease in the weight percent of oxygen is much larger than the percentage increase in elemental oxygen when heavier phenols are formed.

FIMS data for the first LC fraction were obtained without any further separation. Nevertheless, with the aid of certain definite compositional information, which are, that the first fraction of coal liquids produced in fixed-bed reactors contain about 15 weight percent of olefins and saturated compounds, that mono- and di-aromatic compounds are the two major ring systems in this fraction, and that in the present sample not more than two homologous series constitute each column of FIMS data, it was possible to identify all series with reasonable certainty. To illustrate the identification of series in a given column, Column 10 is taken as the example in which are included alkanes, naphthalenes, dibenzothiophenes, binaphthyls, and phenolic compounds. The distribution of relative intensity of molecular ions as a function of carbon number suggest that only two series contribute to this column. The contribution of one series, whose parent compound begins with m/e = 128 to the total relative intensity in the column was 75 percent. Since phenolic compounds were not eluted into this fraction, there are only two possible assignments to the parent compound; an alkane or an aromatic compound. Coal liquids contain mainly higher alkanes at a much lower concentration than aromatics. Therefore, the series beginning with m/e = 128 was assigned to naphthalenes and the other series to alkanes. In a similar manner, homologous series in the other columns were identified. The results suggest that alkanes and cyclic alkanes are cracked in the modified configuration of the fixed-bed reactor, while neutral aromatic compounds are practically unchanged, with the exception of naphthalene. A large increase in the concentration of naphthalene is probably due to its formation from cracking of larger molecules or deoxygenation of naphthols. These possible reactions do not explain why a concentration increase was observed only for naphthalene and not for other aromatic compounds commonly found in fixed-bed samples.

The influence of modified reactor configuration on tar and char yield, gas composition and elemental composition of tar and char are presented in Table 4. In the modified reactor, the tar yield is decreased and the total gas yield is increased. In gaseous products, the increase in the level of C_1-C_8 alkanes is significant. These observations are consistent with some of the reactions induced in the modified reactor, identified based on FIMS data. Cracking of saturated compounds, including alkanes and cyclic alkanes would enhance the total gas production, in particular those of short-chain hydrocarbons.

Compositional Comparison of Pittsburgh No. 8 Coal Liquids Produced in the Entrained-Flow Reactor and the Fixed-Bed Reactor

A primary objective of this comparison was to assess whether coal tars produced in the entrained-flow reactor at elevated temperatures can serve as feedstocks for high energy density fuels. To this end, the first fraction of the LC separation of entrained-flow reactor liquid was analyzed using FIMS, data were reduced and finally, specific chemical structures were assigned to parent members of homologous series. The separation and mass spectral results along with those for the fixed-bed sample are given in Tables 5 and 6, respectively. The pyrolysis temperature in the fixed-bed reactor was 500°C; although the entrained-flow reactor was heated to 850°C, the particle temperature was much less, but at least 100°-150°C higher than 500°C.

Results included in Table 6 are presented in a different format in Figure 1 to highlight the difference in the naphthenic carbon content in the two samples. The first column of this figure contains names of identified compounds along with their structures. In the next two columns, the total number of carbon atoms and naphthenic carbons, respectively, contributed by each structure to the LC fraction-1 of fixed-bed liquid are given. The other two columns contain the same information for the entrained-flow reactor sample. The total number of carbons contributed by aromatic compounds and cyclic alkanes were obtained assuming that on the average that each structure is substituted with three carbon atom side chains. The average number of carbon atoms in normal and branched alkanes was assumed to be 20.

Elemental analysis indicated that the fixed-bed sample was hydrogen rich relative to the EFR sample. According to average molecular parameters derived from the proton NMR spectra, the EFR sample was more aromatic, contained less naphthenic carbons, had a higher concentration of polycyclic aromatic compounds, and the aromatic structures were substituted with shorter alkyl chains relative to the fixed-bed sample. These gross structural features are in agreement with the results of elemental analysis. FIMS results, on the other hand, gave details of structural changes.

Two important compositional differences were reduced concentration of monoaromatic and increased concentration of polycyclic aromatic compounds in the EFR sample relative to the fixed-bed sample. Tetralin, a monoaromatic compound, was probably first changed to butyl benzene and eventually to volatile BTX. Side chains in alkyl benzenes were severely cracked. Elevated temperatures favor ring condensation reactions and in this process certain hydroaromatic compounds were formed. Therefore, EFR samples also contain reasonable amounts of naphthenic carbons, although tetralins and octahydronaphthalenes were substantially depleted at elevated temperatures. However, the total population of naphthenic carbons in the first fraction of fixed-bed sample was higher than in the EFR sample. Also the weight percent of first fraction in the total fixed-bed sample was about 50 percent higher than in the EFR sample. Therefore, coal liquids produced in a fixed-bed reactor have a definite edge as a high energy density fuel feedstock over the EFR liquids.

Compositional Comparison of Coal Liquids Produced from a Fixed-Bed, Fluidized-Bed, and Entrained-Flow Reactors

Coal liquids produced from Pittsburgh No. 8 coal in the fixed-bed and entrained-flow reactors at 650°C and from Illinois No. 6 coal in the fixed-bed and in the fluidized-bed reactors at 500°C were separated using LC and the results are given in Table 7. Unlike for the previously discussed samples, field ionization mass spectral data were obtained for the total sample. Therefore, assignments of chemical structure to the parent compound of each homologous series is based solely on m/e values. Despite this limitation, assignments appear to be reasonable. Results are presented in Tables 8 and 9.

A survey of the composition of fluidized-bed and entrained-flow reactor samples relative to the composition of fixed-bed liquids suggest that cracking of simple hydroaromatic compounds such as tetralins, deoxygenation of simple phenolic compounds, and ring fusion are the reactions induced by rapid pyrolysis both at moderate and elevated temperatures. The ring fusion reaction results in neutral polycyclic aromatic, polycyclic hydroaromatic, and oxygen-containing polycyclic aromatic compounds.

SUMMARY AND CONCLUSIONS

Coal pyrolysis liquids produced by slow heating at moderate temperatures in fixed-bed and modified fixed-bed reactors and by rapid pyrolysis at moderate or elevated temperatures in fluidized-bed or entrained-flow reactors were separated by adsorption chromatography. Pertinent fractions thus generated and total liquids in some cases were analyzed using field ionization mass spectroscopy. The mass spectral data were deconvoluted and each homologous series was associated with a chemical structure. In data analyses for fractions, it was possible to assign definite chemical structures to the parent compound of each series. Identification of components in the total sample is tentative, nevertheless reasonable.

The thrust of this study was to understand compositional differences among coal liquids produced in different reactor configuration and to decide the best configuration for the production of high energy density fuels. In the modified fixed-bed reactor the primary pyrolysis liquid was post-heated to 500°C to understand the influence of heat treatment on liquid quality.

Separation and FIMS results have shown that slow pyrolysis in the modified fixed-bed reactor and rapid pyrolysis both at moderate and elevated temperatures induce some common reactions, in particular deoxygenation of phenolic compounds and cracking of heavier polar compounds.

Rapid pyrolysis depletes the concentration of simple hydroaromatic compounds and alkyl benzenes, and reduces the length of alkyl side chains on aromatic structures. Ring condensation is another reaction induced during rapid pyrolysis and results in polycyclic aromatic, polycyclic hydroaromatic, and oxygen-containing polycyclic aromatic compounds.

Based on compositional data for liquids produced in different reactor configurations, mild gasification liquids produced in the fixed-bed reactor appear to be the suitable feedstock for high energy density fuels.

ACKNOWLEDGEMENT: Funding for this work was provided by the US Dept of Energy, Morgantown Energy Technology Center.

REFERENCES

1(a). Khan, M. R., Fuel Science and Technology International. 5(2), 185, 1987.
1(b). Khan, M. R., Proceedings, International Conference on Coal Science, Elsevier, p. 647, 1987.
2. Farcasiu, M., Fuel. 56(1), 9, (1977).
3. Seshadri, K. S., and D. Cronauer, Fuel. 62(12), 1436, 1983.
4. St. John, G. A., S. E. Buttrill, Jr., and M. Anbar, Organic Chemistry of Coal (Ed. J. Larsen), ACS Symposium Series 71, 223, (1978).
5. Clutter, D. R., L. Petrakis, R. L. Stenger, Jr., and R. K. Jensen, Anal. Chem., 44(8), 1395, (1972).
6. Whitehurst, D. D., S. E. Buttrill, Jr., F. J. Derbyshire, M. Farcasiu, G. A. Odoerfer, and L. R. Rudmik, Fuel, 61, 994, (1982).

TABLE 1. Fractions of Coal Liquids Produced in Fixed-Bed and in the Modified Configuration from Pittsburgh No. 8 and Montana Rosebud Coals

Fraction No.	Weight-Percent in Sample A	B	C	D
1	42.8	42.6	42.8	46.1
2	13.8	4.9	7.5	6.2
3	14.8	24.7	12.1	23.0
4	1.0	2.1	1.4	0.6
5	8.5	12.4	4.3	4.7
6	6.3	7.1	2.5	6.2
Residue	12.8	6.2	27.1	13.5

A -- Pittsburgh No. 8 Fixed-Bed (FB) Reactor
B -- Pittsburgh No. 8 Modified FB Reactor
C -- Montana Rosebud FB Reactor
D -- Montana Rosebud Modified FB Reactor

TABLE 2. Composition of LC Fraction-1 of Montana Rosebud and Pittsburgh No. 8 Coal Liquids Produced in Fixed-Bed and Modified Fixed-Bed Reactors

Compound	MR	MRM	PGH	PGHM
Alkanes and Cyclic Alkanes				
Alkanes, Normal and Branched	4.54	2.10	6.45	4.36
Monocyclic Alkanes	2.39	0.66	3.81	2.69
Tetracyclic Alkanes	2.93	2.07	4.15	2.85
Pentacyclic Alkanes			1.76	0.46
Aromatics				
Benzenes	9.45	9.98	9.43	10.23
Naphthalenes	15.82	19.34	9.63	12.94
Tetralins	12.51	13.76	4.96	4.29
Acenaphthenes/Biphenyls	13.24	13.63	12.59	14.29
Fluorenes	11.87	10.99	9.41	10.53
Anthracenes/Phenanthrenes	11.45	11.08	12.66	12.04
Dibenzothiophenes	0.92	1.12	2.78	1.64
Octahydroanthracenes	8.20	9.72	4.68	4.69
Fluoranthenes	2.80	1.79	8.41	10.52
Dihydropyrenes	--	--	0.74	0.72
Tetrahydro Fluoranthenes	0.80	0.81	1.59	1.44
Chrysenes	3.02	2.89	6.97	6.25

TABLE 3. Composition of LC Fraction-3 of Pittsburgh No. 8 and Montana Rosebud Coal Liquids Produced in Fixed-Bed and Modified Fixed-Bed Reactors (Mole Percent)

Compound	PGH	PGHM	MR	MRM
2-Indenols	3.1	7.0	5.8	7.2
Unidentified	3.8	3.4	2.9	3.0
Hydroxybenzofurans	7.4	11.1	10.9	10.7
Hydroxypyrenes	6.2	4.9	4.7	2.7
Phenols	31.9	27.8	26.1	24.7
Hydroxyphenylnaphthalenes	3.6	4.1	3.2	5.5
Catechols	2.4	1.0	--	--
Phenanthrols	5.2	6.7	7.3	8.3
1-Hydroxy 9,10-Dihydroanthracenes	8.0	9.1	9.48	10.34
Hydroxypentacenes	1.5	1.4	0.74	0.38
Hydroxybiphenyls	10.9	8.5	11.6	9.8
9-Hydroxytetrahydroanthracenes	1.8	1.9	0.2	3.0
Naphthols	9.9	8.2	15.9	12.4
9,10-Dihydroxytetrahydroanthracenes	2.1	3.7	1.3	2.0
Unidentified	1.7	0	--	--

PGH -- Pittsburgh No. 8 Liquid Produced in the FB Reactor
PGHM -- Pittsburgh No. 8 Liquid Produced in the Modified FB Reactor
MR -- Montana Rosebud Liquid Produced in the FB Reactor
MRM -- Montana Rosebud Liquid Produced in the Modified FB Reactor

TABLE 4. Influence of Fixed-Bed Reactor Configuration on Product Composition (Pittsburgh No. 8 Coal) (All Data on Dry Coal Basis)

	Fixed-Bed Reactor	Modified Fixed-Bed Reactor
Wt Sample (g)	50.0	50.0
Total Gas (l)/100 g Dry Coal	10.0	12.5
Char (Wt %)	71.2	72.0
Tar (Wt %)	18.0	9.0
<u>Gas Composition (Vol %)</u>		
H_2	10.51	8.29
CO	4.54	4.46
CO_2	6.81	7.43
H_2S	6.58	5.78
COS	0.16	0.23
H_2O	0.03	0.08
CH_4	48.32	43.22
C_2H_4	1.52	1.79
C_2H_6	9.91	10.80
C_1-C_8	71.10	73.69
<u>Tar Composition (Wt %)</u>		
C	77.62	81.68
H	8.93	8.69
S	0.74	0.93
N	0.94	0.86
O	11.77	7.84
H/C (atomic)	1.38	1.28
Btu/lb	14,926	15,626
<u>Char Composition (as received, Wt %)</u>		
C	78.56	78.73
H	2.89	2.86
N	1.76	1.73
S	1.66	1.71
Ash	10.51	10.77
VM	10.61	11.26
H_2O	0.30	0.81
H/C	0.44	0.44
O (By Difference)	15.13	14.97
Btu/lb	13,121	13,101

TABLE 5. Fractions of Pittsburgh No. 8 Coal Liquids in Fixed-Bed and Entrained-Flow Reactors

Fraction No.	Fixed-Bed	Entrained-Flow Reactor
1	42.8	33.1
2	13.8	3.5
3	14.8	26.5
4	1.0	9.1
5	8.5	8.6
6	6.3	14.0
Residue	12.8	5.2

TABLE 6. Composition in Mole Percent of LC Fraction-1 of Fixed-Bed and Entrained-Flow Reactor Liquids Generated From Pittsburgh No. 8 Coal

Compound	Fixed-Bed	Entrained-Flow
Tetralins	5.0	1.0
Pyrenes/Fluoranthenes	8.4	12.0
Cyclic alkanes	1.8	2.0
Benzenes	4.1	0.9
Dihydropyrenes	9.3	7.4
Tetracyclic alkanes	0.7	4.2
Phenanthrenes	--	9.6
Tetrahydropyrenes	1.6	5.6
Octahydronaphthalenes	12.7	--
Acenaphthylenes	9.4	7.1
Hexahydropyrenes	3.0	--
Octahydrobenzanthracenes	--	6.9
Acenaphthenes	12.6	6.1
Monocyclic alkanes	3.8	--
Benzopyrenes	--	9.3
Naphthalenes	9.6	8.3
Alkanes	6.4	7.5
Binaphthyls	--	0.5
Indenes	4.7	1.8
Chrysenes	6.9	8.3
Unknown	--	1.4

TABLE 7. Fractions of Fixed-Bed and Fluid-Bed (Illinois No. 6) and Fixed-Bed and Entrained-Flow Reactor (Pittsburgh No. 8) Liquids

	Weight Percent in			
Fraction No.	Fixed-Bed Illinois No. 6 500°C	Fluid-Bed Illinois No. 6 500°C	Fixed-Bed Pittsburgh No. 8 650°C	Entrained-Flow Reactor Pittsburgh No. 8 650°C
1	28.6	12.9	39.2	4.7
2	4.6	5.0	14.3	10.3
3	23.8	20.0	14.3	28.3
4	19.7	23.2	5.3	30.0
5	14.1	37.8	9.0	11.4
6	11.29	0.0	5.5	6.2
Residue	9.0	1.1	17.9	9.0

TABLE 8. Relative Weight Percent of Neutral Aromatic and Phenolic Compounds in 500°C Fixed-Bed and Fluid-Bed Liquids (Illinois No. 6 Coal)

Compound	Fixed-Bed	Fluid-Bed
Benzenes	6.1	--
Phenols	11.4	3.6
Catechols/Hydroquinones	--	1.6
Indenes	7.7	--
Naphthalenes	4.5	8.8
Tetralins	7.2	3.8
Benzothiophenes	--	3.1
Naphthols	--	3.7
Acenaphthenes/Biphenyls	10.5	7.5
Fluorenes	9.1	9.7
Hydroxybiphenyls	7.7	--
Octahydronaphthalenes	10.8	--
Anthracenes/Phenanthrenes	--	7.9
Octahydrophenanthrenes	4.5	4.6
Hexylbenzenes	5.1	--
Pyrenes	--	8.6
Dihydropyrenes	--	8.6
Hydroxytetralins	9.3	--
Benzopyrenes	--	2.7
Binaphthyls	1.75	2.6
Chrysenes	--	6.2
Hydroxypentacenes	--	4.2
Dibenzopyrenes	--	2.5
Pentacenes	--	3.1
Dihydrobenzopyrenes	--	2.7

TABLE 9. Composition of Fixed-Bed and Entrained-Flow Reactor Liquids Generated from Pittsburgh No. 8 Coal (650°C)

Compound	Fixed-Bed	Entrained-Flow
Indanes/Tetralins	4.31	0.75
Pyrenes	2.48	5.98
Dihydrobenzanthracenes	1.83	--
Hydroxybenzanthracenes	--	2.20
Hexacenes	--	0.40
Benzenes	5.32	--
Benzofurans	--	1.04
Phenylnaphthalenes or Hydroxypyrenes	4.74	5.76
Dihydroxy Benzanthracenes	--	2.54
Phenols	7.92	0.79
Anthracenes Phenanthrenes Dihydroxytetralins	3.60	5.87
Hydroxyphenyl Naphthalenes	0.99	2.74
Tetrahydropyrenes	1.87	--
Catechols	2.17	--
Acenaphthylenes	5.42	2.84
Phenanthrols	--	1.84
Dihydroxytetrahydro Benzanthracenes	--	3.74
Octahydrotetracenes	0.74	--
Pentacenes	--	0.28
Cyclohexanes	1.06	--
Acenaphthenes/Biphenyls	6.50	3.26
Benzopyrenes	1.01	5.09
Tetrahydronaphthyl Phenyl Ether	0.81	--
Hydroxypentacene	--	1.21
Naphthalenes	9.24	2.04
Hydroxytetrahydroanthracenes	--	1.32
Binaphthyls	1.81	3.69
Unknown	--	1.17
Tribenzopyrenes	0.17	1.39
Indenes	3.90	1.00
Octahydrophenanthracenes/ Dibenzofuran	3.50	--
Dihydroxy Tetrahydro Anthracenes	--	6.41
Bianthryls	--	1.86
Dinaphtho Thiophene	0.58	--

FIGURE 1. Relative Composition of LC Fraction-1 of Fixed-Bed and Entrained-Flow Reactor Coal Liquids (Pittsburgh No. 8)

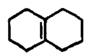
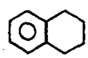
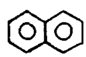
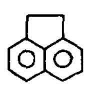
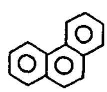
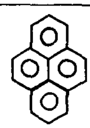
Compound/Structure		Fixed Bed		Entrained-Flow Reactor	
		Total Carbon	Naphthenic Carbon	Total Carbon	Naphthenic Carbon
Octahydronaphthalenes		165.1	101.6	0.0	0.0
Tetralins		65.0	20.0	13.0	4.0
Benzenes		36.9	0.0	8.1	0.0
Naphthalenes		124.8	0.0	107.9	0.0
Acenaphthylenes		141.0	0.0	106.5	0.0
Acenaphthenes		189.0	25.2	91.5	12.2
Phenanthrenes		0.0	0.0	163.2	0.0
Pyrenes		159.6	0.0	228.0	0.0

FIGURE 1. Relative Composition of LC Fraction-1 of Fixed-Bed and Entrained-Flow Reactor Coal Liquids (Pittsburgh No. 8) (Continued)

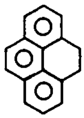
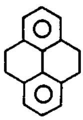
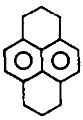
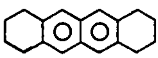
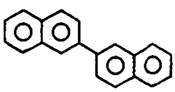
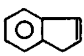
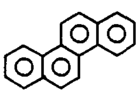
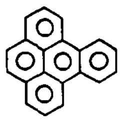
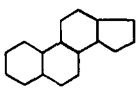
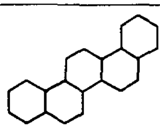
Compound/Structure		Fixed Bed		Entrained-Flow Reactor	
		Total Carbon	Naphthenic Carbon	Total Carbon	Naphthenic Carbon
Dihydropyrenes		176.7	18.6	140.6	14.8
Tetrahydropyrenes		30.4	6.4	106.4	22.4
Hexahydropyrenes		57.0	18.0	0.0	0.0
Octahydrobenzanthracenes		0.0	0.0	144.9	55.2
Binaphthyls		0.0	0.0	7.5	0.0
Indenes		56.4	4.7	21.6	1.8
Chrysenes		144.9	0.0	174.3	0.0

FIGURE 1. Relative Composition of LC Fraction-1 of Fixed-Bed and Entrained-Flow Reactor Coal Liquids (Pittsburgh No. 8) (Continued)

Compound/Structure		Fixed Bed		Entrained-Flow Reactor	
		Total Carbon	Naphthenic Carbon	Total Carbon	Naphthenic Carbon
Benzopyrenes		0.0	0.0	213.9	0.0
Alkanes (n- and branched)		128.0	0.0	150.0	0.0
Monocyclic alkanes		34.2	22.8	0.0	0.0
Tetracyclic alkanes		14.0	11.9	84.0	71.4
Pentacyclic alkanes		45.0	39.6	50.0	44.0
Total		1568	268.8	1811.4	225.8
% Naphthenic Carbon in LC Fraction-1			17.1		12.4
% Naphthenic Carbon in Total Liquid			7.3		4.1